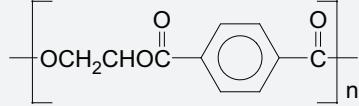
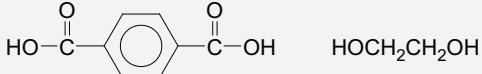


# PET poly(ethylene terephthalate)

PARAMETER	UNIT	VALUE	REFERENCES
<b>GENERAL</b>			
Common name	-	poly(ethylene terephthalate)	
IUPAC name	-	poly(ethylene terephthalate)	
ACS name	-	poly(oxy-1,2-ethanediyl oxycarbonyl-1,4-phenylene carbonyl)	
Acronym	-	PET	
CAS number	-	25038-59-9	
Linear formula			
<b>HISTORY</b>			
Person to discover	-	Whinfield, R J and Dickson, T J	Whinfield, R J and Dickson, T J, US Patent 2,465,319, DuPont, Mar. 22, 1949.
Date	-	1949	
Details	-	first patented by DuPont	
<b>SYNTHESIS</b>			
Monomer(s) structure	-		
Monomer(s) CAS number(s)	-	100-21-0; 107-21-1	
Monomer(s) molecular weight(s)	dalton, g/mol, amu	166.13; 62.07	
Monomer ratio	-	2.676 (72.8:27.2)	
Method of synthesis	-	several processes can be used, including: transesterification, direct esterification, and polycondensation	
Mass average molecular weight, M <sub>w</sub>	dalton, g/mol, amu	19,000-66,000; 29,800-45,800 (recycled)	Romao, W; Freanco, M FF; Bueno, M I M S; De Paoli, M-A, Polym. Test., 29, 879-85, 2010.
Molar volume at 298K	cm <sup>3</sup> mol <sup>-1</sup>	calc.=146.1; 130 (crystalline); 144.5 (amorphous)	
Van der Waals volume	cm <sup>3</sup> mol <sup>-1</sup>	calc.=96.36; 94.2 (crystalline); 94.2 (amorphous)	
Molecular cross-sectional area, calculated	cm <sup>2</sup> x 10 <sup>-16</sup>	14.0	
<b>STRUCTURE</b>			
Crystallinity	%	20-50, 52.5-54.6 (fiber); 85 (oriented film)	Romao, W; Franco, M F; Corilo, Y E; Ebrolin, M N; Spinace, M A S; De Paoli, M-A, Polym. Deg. Stab., 94, 1849-59, 2009; Blundell, D J; Mahendrasingam, A; Martin, C; Fuller, W; MacKerron, D H; Harvie, J L; Oldman, R J; Riekel, C, Polymer, 41, 7793-7802, 2000.
Cell type (lattice)	-	triclinic	
Cell dimensions	nm	a:b:c=0.448-0.456:0.58-0.594:1.071-1.086	
Unit cell angles	degree	$\alpha:\beta:\gamma=98-107:118-119:111-112$	Kinoshita, Y; Nakamura, R; Kitano, Y; Ashida, T, Polym. Prep., 20, 454, 1979.
Number of chains per unit cell	-	1	

# PET poly(ethylene terephthalate)

PARAMETER	UNIT	VALUE	REFERENCES
<b>Crystallite size</b>	nm	27.8-40.8 (fiber)	
<b>Chain conformation</b>	-	nearly planar	
<b>Entanglement molecular weight</b>	dalton, g/mol, amu	1,936	Barany, T; Czigany, T; Karger-Kotsis, J, Prog. Polym. Sci., 35, 1257-87, 2010.
<b>Crystallization temperature</b>	°C	164	Romaao, W; Franco, M F; Corilo, Y E; Ebrlin, M N; Spinace, M A S; De Paoli, M-A, Polym. Deg. Stab., 94, 1849-59, 2009.
<b>Avrami constants, k/n</b>	-	n=2.4-2.7	Lu, X F; Hay, J N, Polymer, 42, 9423-31, 2001.
<b>COMMERCIAL POLYMERS</b>			
<b>Some manufacturers</b>	-	DuPont; Sabic	
<b>Trade names</b>	-	Rynite; PET	
<b>PHYSICAL PROPERTIES</b>			
<b>Density at 20°C</b>	g cm <sup>-3</sup>	1.3-1.4; 1.455 (crystalline); 1.333 (amorphous); 1.47-1.81 (20-55% glass fiber)	
<b>Bulk density at 20°C</b>	g cm <sup>-3</sup>	0.795-0.88	
<b>Color</b>	-	white to gray	
<b>Refractive index, 20°C</b>	-	calc.=1.5392-1.5557; exp.=1.5750	
<b>Birefringence</b>	-	0.0469 (fiber)	Romaao, W; Franco, M F; Corilo, Y E; Ebrlin, M N; Spinace, M A S; De Paoli, M-A, Polym. Deg. Stab., 94, 1849-59, 2009.
<b>Haze</b>	%	0.6	
<b>Odor</b>	-	none	
<b>Melting temperature, DSC</b>	°C	245-265; 254 (20-55% glass fiber)	
<b>Decomposition temperature</b>	°C	285-329	
<b>Storage temperature</b>	°C	<50	
<b>Thermal expansion coefficient, -40 to 160°C</b>	°C <sup>-1</sup>	1.7E-5 (film); 6.55E-4 (melt); 1.1-9.5E-5 (20-55% glass fiber)	Mark, H F; Gaylord, N G, Encyclopedia of Polymer Science, Vol. 11, Interscience, New York, 1969.
<b>Thermal conductivity, melt</b>	W m <sup>-1</sup> K <sup>-1</sup>	calc.=0.1888; exp.=0.147 (melt); 0.29-0.33 (20-55% glass fiber)	
<b>Glass transition temperature</b>	°C	calc.=76-88; exp.=60-85; 60-76 (amorphous)	
<b>Specific heat capacity</b>	J K <sup>-1</sup> kg <sup>-1</sup>	1,170	
<b>Heat of fusion</b>	kJ mol <sup>-1</sup>	24.1	
<b>Maximum service temperature</b>	°C	-60 to 105	
<b>Temperature index (50% tensile strength loss after 20,000 h/5000 h)</b>	°C	140 (20-55% glass fiber)	
<b>Heat deflection temperature at 0.45 MPa</b>	°C	63.9; 240-248 (20-55% glass fiber)	
<b>Heat deflection temperature at 1.8 MPa</b>	°C	61.1; 210-229 (20-55% glass fiber)	
<b>Vicat temperature VST/B/50</b>	°C	77	
<b>Enthalpy of melting</b>	J g <sup>-1</sup>	27	Romaao, W; Franco, M F; Corilo, Y E; Ebrlin, M N; Spinace, M A S; De Paoli, M-A, Polym. Deg. Stab., 94, 1849-59, 2009.

# PET poly(ethylene terephthalate)

PARAMETER	UNIT	VALUE	REFERENCES
Hansen solubility parameters, $\delta_D$ , $\delta_P$ , $\delta_H$	MPa <sup>0.5</sup>	18.7, 6.3, 6.7	
Interaction radius		6.5	
Hildebrand solubility parameter	MPa <sup>0.5</sup>	calc.=14.65-17.15; exp.=17.1-20.8	
Surface tension	mN m <sup>-1</sup>	calc.=38.7-47.3; exp.=39.5-42.1	
Dielectric constant at 100 Hz/1 MHz	-	3.0-3.3/3.2-3.3; 3.2-4.0/3.0-3.9 (20-55% glass fiber)	
Dissipation factor at 100 Hz	E-4	20-25; 50-100 (20-55% glass fiber)	
Dissipation factor at 1 MHz	E-4	30; 110-150 (20-55% glass fiber)	
Volume resistivity	ohm-m	1E13; 1E13 (20-55% glass fiber)	
Surface resistivity	ohm	1E14 (20-55% glass fiber)	
Electric strength K20/P50, d=0.60.8 mm	kV mm <sup>-1</sup>	22-26; 24.5-25.5 (20-55% glass fiber)	
Comparative tracking index, CTI, test liquid A	-	175-400	
Arc resistance	s	120-360	
Power factor	-	0.019	
Coefficient of friction	-	0.45 (film to film); 0.17-0.21 (20-55% glass fiber, self); 0.14 (film to steel); 0.17-0.20 (20-55% glass fiber, steel)	
Permeability to oxygen, 25°C	$m^3 m m^{-2} s^{-1} Pa^{-1} \times 10^{18}$	0.4	Colomiones, G; Ducruet, V; Courgneau, C; Guinault, A; Domenek, S, Polym. Int., 59, 818-26, 2010.
Permeability to water vapor, 25°C	$cm^3 cm cm^{-2} s^{-1} Pa^{-1} \times 10^{12}$	11.3	
Contact angle of water, 20°C	degree	72.0-75.0	Donelli, I; Freddi, G; Niefstrasz, V A; Taddei, Polym. Deg. Stab., 95, 1542-50, 2010.
Surface free energy	mJ m <sup>-2</sup>	44.0	
<b>MECHANICAL &amp; RHEOLOGICAL PROPERTIES</b>			
Tensile strength	MPa	24-41.4; 590 (fiber); 114-189 (20-55% glass fiber)	
Tensile modulus	MPa	2,300; 7,240-17,900 (20-55% glass fiber)	
Tensile stress at yield	MPa	36.5-62.7; 327 (fiber)	
Elongation	%	100-250; 1.6-2.3 (20-55% glass fiber)	
Tensile yield strain	%	4	
Flexural strength	MPa	68.9-78; 172-290 (20-55% glass fiber)	
Flexural modulus	MPa	1,560-2,650; 6,480-17,900 (20-55% glass fiber)	
Compressive strength	MPa	80; 172-241 (20-55% glass fiber)	
Young's modulus	MPa	2,000-2,700	
Izod impact strength, notched, 23°C	J m <sup>-1</sup>	640	
Izod impact strength, notched, -30°C	J m <sup>-1</sup>	190	
Shear strength	MPa	79.0-86.5 (20-55% glass fiber)	
Tenacity (fiber) (standard atmosphere)	cN tex <sup>-1</sup> (daN mm <sup>-2</sup> )	25-95 (35-130)	Fourné, F, Synthetic Fibers. Machines and Equipment Manufacture, Properties. Carl Hanser Verlag, 1999.

# PET poly(ethylene terephthalate)

PARAMETER	UNIT	VALUE	REFERENCES
Tenacity (wet fiber, as % of dry strength)	%	95-100	Fourne, F, Synthetic Fibers. Machines and Equipment Manufacture, Properties. Carl Hanser Verlag, 1999.
Fineness of fiber (titer)	dtex	0.6-44	Fourne, F, Synthetic Fibers. Machines and Equipment Manufacture, Properties. Carl Hanser Verlag, 1999.
Length (elemental fiber)	mm	38-200, filament	Fourne, F, Synthetic Fibers. Machines and Equipment Manufacture, Properties. Carl Hanser Verlag, 1999.
Abrasion resistance (ASTM D1044)	mg/1000 cycles	30-44	
Poisson's ratio	-	0.421-0.430; 0.39-0.41 (20-55% glass fiber)	
Rockwell hardness	-	R110; M95-100 (20-55% glass fiber); R120 (20-55% glass fiber)	
Shrinkage	%	0.7-1.2; 0.18-0.35 (20-55% glass fiber, flow); 0.7-0.9 (20-55% glass fiber, transverse)	
Intrinsic viscosity, 25°C	dl g <sup>-1</sup>	0.75-0.84	
Melt index, 230°C/3.8 kg	g/10 min	7	
Water absorption, 24h at 23°C	%	0.04-0.14 (24 h); 0.6 (eq)	
Moisture absorption, equilibrium 23°C/50% RH	%	0.35	
<b>CHEMICAL RESISTANCE</b>			
Acid dilute/concentrated	-	good/fair	
Alcohols	-	good/fair	
Alkalies	-	poor	
Aliphatic hydrocarbons	-	good	
Aromatic hydrocarbons	-	good	
Esters	-	fair-poor	
Greases & oils	-	good	
Halogenated hydrocarbons	-	poor	
Ketones	-	fair	
Good solvent	-	DMSO (hot), halogenated aliphatic carboxylic acids, nitrobenzene, phenol	
Non-solvent	-	aliphatic alcohols, carboxylic esters, chlorinated hydrocarbons, ether, hydrocarbons, ketones	
<b>FLAMMABILITY</b>			
Ignition temperature	°C	390	
Autoignition temperature	°C	508	
Limiting oxygen index	% O <sub>2</sub>	20-23; 20 (20-55% glass fiber)	
Char at 500°C	%	5.1	Lyon, R E; Walters, R N, J. Anal. Appl. Pyrolysis, 71, 27-46, 2004.
Heat of combustion	J g <sup>-1</sup>	24,130	Walters, R N; Hacket, S M; Lyon, R E, Fire Mater., 24, 5, 245-52, 2000.
Volatile products of combustion	-	CO, CO <sub>2</sub> , acrolein, formaldehyde, ethanol, methanol, acetic acid, acetone	
UL rating	-	HB (20-55% glass fiber); V-0 (20-55% glass fiber and flame retardant)	

# PET poly(ethylene terephthalate)

PARAMETER	UNIT	VALUE	REFERENCES
<b>WEATHER STABILITY</b>			
<b>Spectral sensitivity</b>	nm	290-325; 270-325	Yang, J; Xia, Z; Kong, F; Ma, X, Polym. Deg. Stab., 95, 53-8, 2010.
<b>Activation wavelengths</b>	nm	305, 325	Yang, J; Xia, Z; Kong, F; Ma, X, Polym. Deg. Stab., 95, 53-8, 2010.
<b>Excitation wavelengths</b>	nm	280, 320, 344, 357; 300 and 330	Yang, J; Xia, Z; Kong, F; Ma, X, Polym. Deg. Stab., 95, 53-8, 2010.
<b>Emission wavelengths</b>	nm	370, 389, 405, 425, 460; 328 and 387+460	Yang, J; Xia, Z; Kong, F; Ma, X, Polym. Deg. Stab., 95, 53-8, 2010.
<b>Important initiators and accelerators</b>	-	ferrocene, cobalt octoates and naphthenates, compounds containing aromatic keto-ester groups	
<b>Products of degradation</b>	-	radicals, crosslinks, hydroperoxides, hydroxyl and carbonyl groups, CO, CO <sub>2</sub>	
<b>Stabilizers</b>	-	UVA: 2-hydroxy-4-octyloxybenzophenone; 2-hydroxy-4-methoxybenzophenone; 2,4-dihydroxybenzophenone; 2,2',4,4'-tetrahydroxybenzophenone; 2,2'-dihydroxy-4-methoxybenzophenone; 2-(2H-benzotriazol-2-yl)-p-cresol; 2-benzotriazol-2-yl-4,6-di-tert-butylphenol; 2-(2H-benzotriazole-2-yl)-4,6-di-tert-pentylphenol; 2-(2H-benzotriazole-2-yl)-4-(1,1,3,3-tetraethylbutyl)phenol; 2-(2H-benzotriazol-2-yl)-4,6-bis(1-methyl-1-phenylethyl)phenol; 2,2'-methylenebis(6-(2H-benzotriazol-2-yl)-4-1,1,3,3-tetramethylbutyl)phenol; 2-(2H-benzotriazol-2-yl)-6-dodecyl-4-methylphenol, branched & linear; 2-(2H-benzotriazol-2-yl)-4,6-bis(1-methyl-1-phenylethyl)phenol; 2,4-di-tert-butyl-6-(5-chloro-2H-benzotriazole-2-yl)-phenol; 2-(3-sec-butyl-5-tert-butyl-2-hydroxyphenyl)benzotriazole; 2-[4-[(2-hydroxy-3-(2'-ethyl)hexyl)oxy]-2-hydroxyphenyl]-4,6-bis(2,4-dimethylphenyl)-1,3,5-triazine; 2-(4,6-diphenyl-1,3,5-triazin-2-yl)-5-hexyloxy-phenol; 2-[4,6-bis(2,4-dimethylphenyl)-1,3,5-triazin-2-yl]-5-(octyloxy)phenol; (2-ethylhexyl)-2-cyano-3,3-diphenylacrylate; 1,3-bis-[(2'-cyano-3',3'-diphenylacryloyl)oxy]-2,2-bis-{{[2'-cyano-3',3'-diphenylacryloyl)oxy]methyl}-propane; propano-dioic acid, [(4-methoxyphenyl)-methylen]-dimethyl ester; 2,2'-(1,4-phenylene)bis[4H-3,1-benzoxazin-4-one]; Screeners: carbon black, zinc oxide; Acid scavenger: hydrotalcite; HAS: 1,3,5-triazine-2,4,6-triamine, N,N''[1,2-ethane-diyl-bis[[4,6-bis[butyl(1,2,6,6-pentamethyl-4-piperidinyl)amino]-1,3,5-triazine-2-yl]imino]-3,1-propanediyl]bis[N',N"-dibutyl-N',N"-bis(1,2,2,6,6-pentamethyl-4-piperidinyl)-; decanedioic acid, bis(2,2,6,6-tetramethyl-1-(octyloxy)-4-piperidinyl)ester, reaction products with 1,1-dimethylethylhydroperoxide and octane; bis(1,2,2,6,6-pentamethyl-4-piperidyl)sebacate + methyl-1,2,2,6,6-pentamethyl-4-piperidyl sebacate; alkenes, C20-24-.alpha.-, polymers with maleic anhydride, reaction products with 2,2,6,6-tetramethyl-4-piperidinamine; 1,6-hexanediamine, N, N'-bis(2,2,6,6-tetramethyl-4-piperidinyl)-, polymers with 2,4-dichloro-6-(4-morpholinyl)-1,3,5-triazine; 1,6-hexanediamine, N,N'-bis(2,2,6,6-tetramethyl-4-piperidinyl)-, polymers with morpholine-2,4,6-trichloro-1,3,5-triazine reaction products, methylated; Phenolic antioxidants: ethylene-bis(oxyethylene)-bis(3-(5-tert-butyl-4-hydroxy-m-tolyl)-propionate); N,N'-hexane-1,6-diylbis(3-(3,5-di-tert-butyl-4-hydroxy-phenylpropionamide)); 3,3',3',5,5',5'-hexa-tert-butyl-a,a',a'-(mesitylene-2,4,6-triyl)tri-p-cresol; 1,3,5-tris(3,5-di-tert-butyl-4-hydroxybenzyl)-1,3,5-triazine-2,4,6(1H,3H,5H)-trione; Phosphite: bis-(2,4-di-tert-butylphenol) pentaerythritol diphosphite; tris (2,4-di-tert-butylphenyl)phosphite; phosphoric acid, (2,4-di-butyl-6-methylphenyl)ethylester; distearyl pentaerythritol diphosphite; Optical brightener: 2,2'-(2,5-thiophenediyl)bis(5-tert-butylbenzoxazole)	

# PET poly(ethylene terephthalate)

PARAMETER	UNIT	VALUE	REFERENCES
<b>BIODEGRADATION</b>			
Typical biodegradants	-	abiotic hydrolysis is the most important reaction for initiating the environmental degradation of poly(ethylene terephthalate). Also cutinases and carboxylesterases have both shown the potential to hydrolyze polyester bonds similarly to lipases	Donelli, I; Freddi, G; Niefstrasz, V A; Taddei, Polym. Deg. Stab., 95, 1542-50, 2010.
Stabilizers	-	2,4,4'-trichloro-2'-hydroxydiphenyl ether, N-hexyl-N'-(4-vinylbenzyl)-4,4'-bipyridinium bromide chloride	
<b>TOXICITY</b>			
HMIS: Health, Flammability, Reactivity rating	-	1/1/0	
Carcinogenic effect		not listed by ACGIH, NIOSH, NTP	
Oral rat, LD <sub>50</sub>	mg kg <sup>-1</sup>	>10,000	
<b>ENVIRONMENTAL IMPACT</b>			
Cradle to grave non-renewable energy use	MJ/kg	69.7-85.5	
Cradle to pellet greenhouse gasses	kg CO <sub>2</sub> , kg <sup>-1</sup> resin	2.5-3.5	
<b>PROCESSING</b>			
Typical processing methods	-	blow molding, extrusion, injection blow molding, injection molding, monofilament extrusion	
Preprocess drying: temperature/time/residual moisture	°C/h/%	110-175/2-16/0.003-0.02	
Processing temperature	°C	260-300	
Additives used in final products	-	Fillers: antimony doped tin oxide, aramid, carbon black, carbon fiber, clays, fly ash, glass fiber, glass spheres, mica, montmorillonite, multiwalled carbon nanotubes, silica, talc, titanium dioxide, wollastonite; Antistatics: antimony-doped tin oxide, carbon nanotubes, polyaniline, polyisobutylphthalene; Antiblocking: calcium carbonate, diatomaceous earth, silicone fluid, spherical silicone resin, synthetic silica; Release: calcium stearate, fluorine compounds, glycerol bisstearate, pentaerythritol ester, silane modified silica, zinc stearate; Slip: spherical silica, silicone oil	
Applications	-	automotive, bottles, brush bristles, composites, electrical, fiber, film, housings, housewares, lighting, medical (orthopedic bandages, artificial kidneys, sutures, artificial tendons, cardiovascular implants), motor parts, packaging, plumbing, power tools, sporting goods, support brackets, textiles	
Outstanding properties	-	high strength, stiffness, excellent, dimensional stability, outstanding chemical, excellent flow characteristics, and heat resistance, and good electrical properties	
<b>ANALYSIS</b>			
FTIR (wavenumber-assignment)	cm <sup>-1</sup> /-	detailed assignment for amorphous and crystalline in ref.	Donelli, I; Freddi, G; Niefstrasz, V A; Taddei, Polym. Deg. Stab., 95, 1542-50, 2010.
NMR (chemical shifts)	ppm	H NMR: terephthalic acid – 4.80; ethylene glycol – 8.13; isophthalic acid – 8.71, 8.29, 7.60; diethylene glycol – 4.64, 4.13	Romaao, W; Franco, M F; Corilo, Y E; Ebrlin, M N; Spinace, M A S; De Paoli, M-A, Polym. Deg. Stab., 94, 1849-59, 2009.
x-ray diffraction peaks	degree	21.3	Sun, B; Lu, Y; Ni, H; Wang, C, Polymer, 39, 1, 159-63, 1998.